(12)

FINAL TECHNICAL SUMMARY REPORT

for the period

1 October 1981 - 30 September 1982

THERMODYNAMICS OF ORGANIC COMPOUNDS

Bartlesville Energy Technology Center
Department of Energy
Bartlesville, Oklahoma

Research sponsored by:

Air Force Office of Scientific Research (NA)
Department of the Air Force

Contract No. AFOSR-ISSA 82-00012
Project No. 2308/A2

Approved for public release;
distribution unlimited.

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE	READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER AFOSR-TR- 83-0047	2. GOVT ACCESSION NO. AD-A125022 / 3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) THERMODYNAMICS OF ORGANIC COMPOUNDS,	5. TYPE OF REPORT & PERIOD COVERED Final Report 1 Oct 81 - 30 Sep 82,
	6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) B E GAMMON, N K SMITH	8. CONTRACT OR GRANT NUMBER(s) AFOSR-ISSA-82-00012
9. PERFORMING ORGANIZATION NAME AND ADDRESS BARTLESVILLE ENERGY TECHNOLOGY CENTER DEPARTMENT OF ENERGY BARTLESVILLE, OK 74005	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS 2308/A2 61102F
11. CONTROLLING OFFICE NAME AND ADDRESS AIR FORCE OFFICE OF SCIENTIFIC RESEARCH/NA BOLLING AFB, DC 20332	12. REPORT DATE November 1982
	13. NUMBER OF PAGES 12
14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office)	15. SECURITY CLASS. (of this report) UNCLASSIFIED
	15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

RAMJET FUELS
ENTHALPY OF COMBUSTION
VAPOR PRESSURE
HEAT CAPACITY
ALKYLINDANS
ALKYLNAPHTHALENES
HEPTACYCLOTETRADECANE

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

This research program consisted of an integrated and interrelated effort of basic and applied research in chemical thermodynamics and thermochemistry. Knowledge of variation of physical and thermodynamic properties with molecular structure was used to select compounds for study that because of high ring strain or unusual steric effects may have good energy characteristics per unit volume or per unit mass and thus be useful in the synthesis of high energy fuels. These materials were synthesized, and their

DD FORM 1 JAN 73 1473 EDITION OF 1 NOV 65 IS OBSOLETE

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

thermodynamic properties were evaluated. In cooperation with researchers at Wright-Patterson Air Force Base, ramjet fuels currently in use were subjected to careful thermodynamic evaluation by measurements of heat capacity, enthalpy of combustion and vapor pressure. During the last year of this effort, seven kerosene-type fuels produced by British Petroleum and seven jet fuels produced from shale oil were studied.

FINAL TECHNICAL SUMMARY REPORT

THERMODYNAMICS OF ORGANIC COMPOUNDS

* * * * * * * * * * * * *

Bartlesville Energy Technology Center
Department of Energy
Bartlesville, Oklahoma

Project Director: W. D. Good

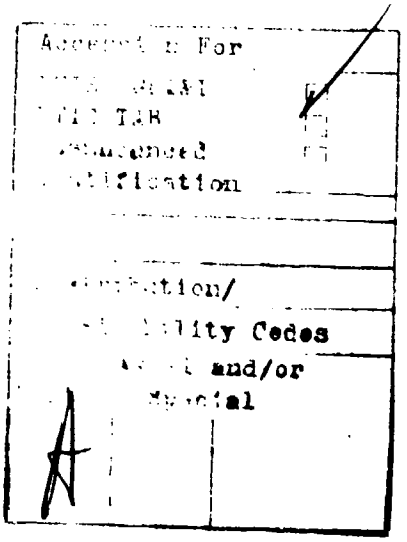
Report* prepared by:

B. E. Gammon
N. K. Smith

W. D. Good, Division Director
Edward J. Lievens, Jr., Acting Director

* Synthesis and purification of research samples were provided by Professor E. J. Eisenbrɛ ɯn, Oklahoma State University. Samples were produced by purchase agreement for this project.

TABLE OF CONTENTS



FOREWORD

This research program consists of an integrated and interrelated effort of basic and applied research in chemical thermodynamics and thermochemistry. Knowledge of variation of physical and thermodynamic properties with molecular structure is used to select compounds for study that because of high ring strain or unusual steric effects may have good energy characteristics per unit volume or per unit mass and thus be useful in the synthesis of high energy fuels. These materials are synthesized, and their thermodynamic properties are evaluated. In cooperation with researchers at Wright-Patterson Air Force Base, ramjet fuels currently in use are subjected to careful thermodynamic evaluation by measurements of heat capacity, enthalpy of combustion and vapor pressure.

ABSTRACT

The research effort continues to be focused on high-density/high-energy hydrocarbons. In cooperation with researchers at Wright-Patterson Air Force Base, heats of combustion are measured for constituents of current ramjet fuels and for finished fuels; meanwhile, pure hydrocarbons were synthesized for heat-of-combustion measurements to determine unusual steric or strain energies which may contribute to design of high-energy/high-density fuels of the future.

Seven kerosene-type fuels produced by British Petroleum and seven jet fuels produced from shale oil were studied during the current reporting period. Synthesis and purification of hydrocarbons were continued at Oklahoma State University; two ethylindans have been received and are being prepared for study.

RESEARCH PROGRESS

1. ENTHALPY OF COMBUSTION OF FUELS

A set of seven kerosene-type fuels produced by British Petroleum, designated BP···, and a set of seven jet fuels produced from shale oil, designated JP···, were studied by bomb calorimetry at the request of researchers at Wright-Patterson Air Force Base. The procedures used and the results from these studies are given below. The letters BP were added to the prefix for the so-designated samples to be consistent with designations received by phone from Don Potter in the spring of 1982 when he gave the 15° C densities and the hydrogen and sulfur analysis for these materials. Otherwise the designations were taken from the labels on the sample bottles from Wright-Patterson Air Force Base dated January 1982.

Experimental procedures used for the combustion calorimetry of hydrocarbons by this laboratory have been described;[1,2] although the fuels used in these experiments are not hydrocarbons, essentially the same procedures were used. Rotating-bomb calorimeter BMR II[3] and platinum-lined bomb Pt-3b[4] were used, without bomb rotation. Fragile, flexible borosilicate glass ampoules[2,5] were used to confine the volatile samples. For each experiment, 1 cm^3 of water was added to the bomb. In one experiment on each sample, the air was flushed from the bomb before charging with pure oxygen; in all the other experiments the bomb was charged with oxygen without flushing. After one of the combustion experiments for each sample, the CO_2 was recovered in weighing tubes to provide missing information and independent checks on the elemental analyses. After the bomb was discharged, the liquid content was quantitatively transferred to an Erlenmeyer flask, and it was then titrated with standard sodium hydroxide solution to determine the total acid formed in the combustion reaction (either sulfuric acid, nitric acid, or a mixture of these two acids). The relative amounts of sulfuric and nitric acids were determined by subtracting the calculated amount of sulfuric acid from the measured total amount of acid; the amount of sulfuric acid was calculated from the empirical formula of the sample and the sample mass.

Results of all of the experiments are given in Tables 1 through 7. Values of $\Delta E_c^\circ/m$ in these tables refer to the reaction of unit mass of sample according to the following equation:

$$C_aH_bS_e(liq) + [a + b/4 + 3e/2]\ O_2(g) + (ne + e - b/2)\ H_2O(liq) =$$

$$a\ CO_2(g) + e(H_2SO_4 \cdot nH_2O)(liq). \qquad (1)$$

A more useful value computed from the combustion experiments may be the value of the energy of the reaction in which water appears in the combustion products in the gaseous state, and sulfur, if present, appears as gaseous sulfur dioxide:

$$C_aH_bS_e(liq) + [a + b/4 + e]\ O_2(g) =$$

$$a\ CO_2(g) + b/2\ H_2O(g) + e\ SO_2(g). \qquad (2)$$

Values of the enthalpies of formation of gaseous SO_2, aqueous H_2SO_4, gaseous H_2O and liquid H_2O were used to convert the average values of the energy of reaction (Tables 1 through 7, Equation 1) to the energy of reaction (Table 8, Equation 2).

The empirical formulas shown in Table 8 were derived from the analysis for sulfur and the ASTM wide-line NMR analysis for hydrogen from Don Potter at Wright-Patterson Air Force Base and from our analysis for carbon. The percentages of elements usually summed to 100 to within 0.1 percent for each compound; one noted exception was sample JP-4-S-A (UN-81-141) which had a sum of 0.45 percent low. In Table 8 the densities at 15° C were supplied by Don Potter, and the values at 25° C were determined as auxiliary information to the bomb calorimetry.

A simple correlation of the values of $\Delta E_c^\circ/m$ in column five of Table 8 was made as follows:

$$\Delta E_c^\circ/m = A + B(\text{pct H}) \qquad (3)$$

$$A = -8400.24 \pm 61.83$$

$$B = 436.047 \pm 4.437$$

where the weight percent hydrogen (pct H) can be determined from the empirical formulas of Table 8. The deviations from the equation are shown in column six of Table 8 where the largest value is 0.25 percent too positive.

TABLE 1. Summary of combustion experiments for BP-IP-1 and BP-IP-2 fuels[a]

(cal_{th} = 4.184 J)

Sample	BP-IP-1			BP-IP-2		
Experiment number	1	2	3	1	2	3
m'(fuel)/g	0.668625	0.675561	0.675463	0.679541	0.679461	0.679908
m''(auxiliary oil)/g	0.054757	0.048261	0.053966	0.053499	0.045640	0.050006
m'''(fuse)/g	0.000997	0.000932	0.001071	0.000761	0.000901	0.000990
$n^i(H_2O)$/mol	0.05535	0.05535	0.05535	0.05535	0.05535	0.05535
$\Delta t_c/K = (t_f - t_i + \Delta t_{corr})/K$	1.99784	2.00272	2.01882	2.02150	2.00293	2.01697
ϵ(calor)$(-\Delta t_c)/cal_{th}$	-8005.89	-8025.43	-8089.95	-8100.69	-8026.28	-8082.54
ϵ(cont)$(-\Delta t_c)/cal_{th}$[b]	-8.69	-8.69	-8.84	-8.77	-8.76	-8.74
$\Delta E_{ign}/cal_{th}$	0.18	0.18	0.18	0.18	0.18	0.18
$\Delta E_{dec}(HNO_3)/cal_{th}$	0.00	13.43	13.77	0.00	14.78	13.92
ΔE(corr to std states)$/cal_{th}$[c]	2.47	2.39	2.42	2.52	2.39	2.42
$\{-m''(\Delta E_c^\circ/m)$(auxiliary oil)$\}/cal_{th}$	602.56	531.09	593.87	588.72	502.24	550.29
$\{-m'''(\Delta E_c^\circ/m)$(fuse)$\}/cal_{th}$	4.04	3.77	4.34	3.08	3.65	4.01
$\{m'(\Delta E_c^\circ/m)$(fuel)$\}/cal_{th}$	-7405.33	-7403.26	-7404.21	-7514.96	-7511.80	-7520.46
$\{(\Delta E_c^\circ/m)$(fuel)$\}/cal_{th}\ g^{-1}$	-11075.45	-11077.10	-11080.13	-11058.88	-11055.52	-11060.99
$\{(\Delta E_c^\circ/m)$(fuel)$\}/cal_{th}\ g^{-1}$	-11077.56 ± 1.37 (mean and standard deviation of the mean)			-11058.46 ± 1.59		

[a] The symbols and abbreviations of this table are those of W. N. Hubbard et al, *Experimental Thermochemistry*, Chap. 5, pp. 75-128. F. D. Rossini, editor. Interscience: 1956.

[b] ϵ^i(cont)$(t_i - 298.15\ K) + \epsilon^f$(cont)$(298.15\ K - t_f + \Delta t_{corr})$.

[c] Items 81 to 85, 87 to 90, 93 and 94 of the computation form of Hubbard et al (footnote a).

TABLE 2. Summary of combustion experiments for BP-IP-3 and BP-IP-4 fuels[a]

(cal_{th} = 4.184 J)

Sample	BP-IP-3			BP-IP-4		
Experiment number	1	2	3	1	2	3
m'(fuel)/g	0.667804	0.666184	0.663254	0.667251	0.664744	0.660514
m''(auxiliary oil)/g	0.053619	0.060042	0.065139	0.060106	0.061745	0.060458
m'''(fuse)/g	0.001007	0.000826	0.000942	0.001083	0.000801	0.001049
$n^i(H_2O)$/mol	0.05535	0.05535	0.05535	0.05535	0.05535	0.05535
$\Delta t_c/K = (t_f - t_i + \Delta t_{corr})/K$	1.98547	2.00253	2.00862	2.00254	2.00319	1.98846
ϵ(calor)$(-\Delta t_c)/cal_{th}$	-7956.31	-8024.68	-8049.08	-8024.72	-8027.33	-7968.32
ϵ(cont)$(-\Delta t_c)/cal_{th}$[b]	-8.55	-8.78	-8.73	-8.70	-8.70	-8.69
$\Delta E_{ign}/cal_{th}$	0.18	0.18	0.18	0.18	0.18	0.18
$\Delta E_{dec}(HNO_3)/cal_{th}$	0.00	14.62	14.27	0.00	13.14	12.93
ΔE(corr to std states)$/cal_{th}$[c]	2.47	2.40	2.42	2.51	2.43	2.41
$\{-m''(\Delta E_c^\circ/m)$(auxiliary oil)$\}/cal_{th}$	590.05	660.72	716.81	661.43	679.47	665.30
$\{-m'''(\Delta E_c^\circ/m)$(fuse)$\}/cal_{th}$	4.08	3.34	3.81	4.38	3.24	4.25
$\{m'(\Delta E_c^\circ/m)$(fuel)$\}/cal_{th}$	-7368.08	-7352.20	-7320.32	-7364.92	-7337.57	-7291.94
$\{(\Delta E_c^\circ/m)$(fuel)$\}/cal_{th}\ g^{-1}$	-11033.29	-11036.30	-11036.96	-11037.71	-11038.19	-11039.81
$\{(\Delta E_c^\circ/m)$(fuel)$\}/cal_{th}\ g^{-1}$	-11035.52 ± 1.13 (mean and standard deviation of the mean)			-11038.57 ± 0.64		

[a] The symbols and abbreviations of this table are those of W. N. Hubbard et al, *Experimental Thermochemistry*, Chap. 5, pp. 75-128. F. D. Rossini, editor. Interscience: 1956.

[b] ϵ^i(cont)$(t_i - 298.15\ K) + \epsilon^f$(cont)$(298.15\ K - t_f + \Delta t_{corr})$.

[c] Items 81 to 85, 87 to 90, 93 and 94 of the computation form of Hubbard et al (footnote a).

TABLE 3. Summary of combustion experiments for BP-IP-5 and BP-IP-6 fuels[a]

(cal_{th} = 4.184 J)

Sample	BP-IP-5			BP-IP-6		
Experiment number	1	2	3	1	2	3
m'(fuel)/g	0.648128	0.645746	0.608922	0.644414	0.611948	0.609626
m''(auxiliary oil)/g	0.061152	0.081022	0.131735	0.069067	0.121556	0.118052
m'''(fuse)/g	0.000952	0.001063	0.001104	0.000980	0.001356	0.001128
$n^i(H_2O)$/mol	0.05535	0.05535	0.05535	0.05535	0.05535	0.05535
$\Delta t_c/K = (t_f - t_i + \Delta t_{corr})/K$	1.94828	2.00115	2.03850	1.94755	2.00696	1.99156
ϵ(calor)$(-\Delta t_c)/cal_{th}$	-7807.28	-8019.15	-8168.84	-7804.38	-8042.45	-7980.72
ϵ(cont)$(-\Delta t_c)/cal_{th}$[b]	-8.49	-8.76	-8.88	-8.41	-8.81	-8.66
$\Delta E_{ign}/cal_{th}$	0.18	0.18	0.18	0.18	0.18	0.18
$\Delta E_{dec}(HNO_3)/cal_{th}$	0.00	12.51	13.55	0.00	13.03	13.98
ΔE(corr to std states)$/cal_{th}$[c]	2.48	2.48	2.53	2.55	2.55	2.52
$\{-m''(\Delta E_c^\circ/m)$(auxiliary oil)$\}/cal_{th}$	672.94	891.60	1449.67	760.04	1337.65	1299.09
$\{-m'''(\Delta E_c^\circ/m)$(fuse)$\}/cal_{th}$	3.85	4.30	4.47	3.97	5.49	4.57
$\{m'(\Delta E_c^\circ/m)$(fuel)$\}/cal_{th}$	-7136.32	-7116.84	-6707.32	-7046.05	-6692.36	-6669.04
$\{(\Delta E_c^\circ/m)$(fuel)$\}/cal_{th}\ g^{-1}$	-11010.66	-11021.10	-11015.08	-10934.04	-10936.16	-10939.56
$\{(\Delta E_c^\circ/m)$(fuel)$\}/cal_{th}\ g^{-1}$	-11015.61 ± 3.02 (mean and standard deviation of the mean)			-10936.58 ± 1.61		

[a] The symbols and abbreviations of this table are those of W. N. Hubbard et al, *Experimental Thermochemistry*, Chap. 5, pp. 75-128. F. D. Rossini, editor. Interscience: 1956.

[b] ϵ^i(cont)$(t_i - 298.15\ K) + \epsilon^f$(cont)$(298.15\ K - t_f + \Delta t_{corr})$.

[c] Items 81 to 85, 87 to 90, 93 and 94 of the computation form of Hubbard et al (footnote a).

TABLE 4. Summary of combustion experiments for BP-IP-7 and BP-IP-9 fuels[a]

(cal_{th} = 4.184 J)

Sample	BP-IP-7		BP-IP-6		
Experiment number	1	2	1	2	3
m'(fuel)/g	0.607569	0.676230	0.639897	0.689602	0.610359
m''(auxiliary oil)/g	0.066801	0.054959	0.083057	0.050499	0.130568
m'''(fuse)/g	0.000796	0.001023	0.000919	0.001108	0.001101
$n^i(H_2O)$/mol	0.05535	0.05535	0.05535	0.05535	0.05535
$\Delta t_c/K = (t_f - t_i + \Delta t_{corr})/K$	1.84351	2.00214	1.96109	2.01902	2.01545
$\varepsilon(calor)(-\Delta t_c)/cal_{th}$	-7387.46	-8023.14	-7858.61	-8054.69	-8076.45
$\varepsilon(cont)(-\Delta t_c)/cal_{th}$[b]	-7.93	-8.73	-8.51	-8.70	-8.86
$\Delta E_{ign}/cal_{th}$	0.18	0.18	0.18	0.18	0.18
$\Delta E_{dec}(HNO_3)/cal_{th}$	0.00	12.50	0.00	12.77	13.24
$\Delta E_{(corr\ to\ std\ states)}/cal_{th}$[c]	2.37	2.55	2.68	2.69	2.66
$\{-m''(\Delta E_c^\circ/m)(auxiliary\ oil)\}/cal_{th}$	735.11	604.79	913.99	555.71	1436.82
$\{-m'''(\Delta E_c^\circ/m)(fuse)\}/cal_{th}$	3.22	4.14	3.72	4.49	4.46
$\{m'(\Delta E_c^\circ/m)(fuel)\}/cal_{th}$	-6654.51	-7407.71	-6946.55	-7487.55	-6627.95
$\{(\Delta E_c^\circ/m)(fuel)\}/cal_{th}\ g^{-1}$	-10952.69	-10954.42	-10855.74	-10857.79	-10859.08
$\{(\Delta E_c^\circ/m)(fuel)\}/cal_{th}\ g^{-1}$	-10953.55 ± 0.86 (mean and standard deviation of the mean)		-10857.54 ± 0.97		

[a] The symbols and abbreviations of this table are those of W. N. Hubbard et al, *Experimental Thermochemistry*, Chap. 5, pp. 75-128. F. D. Rossini, editor. Interscience: 1956.

[b] $\varepsilon^i(cont)(t_i - 298.15\ K) + \varepsilon^f(cont)(298.15\ K - t_f + \Delta t_{corr})$.

[c] Items 81 to 85, 87 to 90, 93 and 94 of the computation form of Hubbard et al (footnote a).

TABLE 5. Summary of combustion experiments for JP-10 and JP-7P-TK-WA-10 fuels[a]

(cal_{th} = 4.184 J)

Sample	JP-10			JP-7P-TK-WA-10		
Experiment number	1	2	3	1	2	3
m'(fuel)/g	0.579676	0.572309	0.629061	0.663507	0.662551	0.672399
m''(auxiliary oil)/g	0.069644	0.171760	0.116749	0.054313	0.056088	0.046723
m'''(fuse)/g	0.000838	0.001095	0.001116	0.000999	0.001033	0.001243
$n^i(H_2O)$/mol	0.05535	0.05535	0.05535	0.05535	0.05535	0.05535
$\Delta t_c/K = (t_f - t_i + \Delta t_{corr})/K$	1.74082	2.00553	2.00572	1.99218	1.99749	1.99972
$\varepsilon(calor)(-\Delta t_c)/cal_{th}$	-6975.96	-8036.71	-8037.46	-7983.22	-8004.51	-8013.42
$\varepsilon(cont)(-\Delta t_c)/cal_{th}$[b]	-7.40	-8.75	-8.80	-8.61	-8.75	-8.64
$\Delta E_{ign}/cal_{th}$	0.18	0.18	0.18	0.18	0.18	0.18
$\Delta E_{dec}(HNO_3)/cal_{th}$	0.00	14.63	12.42	0.00	12.40	12.39
$\Delta E_{(corr\ to\ std\ states)}/cal_{th}$[c]	2.45	2.76	2.81	2.39	2.32	2.32
$\{-m''(\Delta E_c^\circ/m)(auxiliary\ oil)\}/cal_{th}$	766.39	1890.11	1284.66	597.69	617.21	514.16
$\{-m'''(\Delta E_c^\circ/m)(fuse)\}/cal_{th}$	3.39	4.43	4.52	4.04	4.18	5.03
$\{m'(\Delta E_c^\circ/m)(fuel)\}/cal_{th}$	-6210.95	-6133.35	-6741.67	-7387.53	-7376.97	-7487.98
$\{(\Delta E_c^\circ/m)(fuel)\}/cal_{th}\ g^{-1}$	-10714.51	-10716.84	-10717.05	-11134.06	-11134.19	-11136.20
$\{(\Delta E_c^\circ/m)(fuel)\}/cal_{th}\ g^{-1}$	-10716.13 ± 0.82 (mean and standard deviation of the mean)			-11134.82 ± 0.69		

[a] The symbols and abbreviations of this table are those of W. N. Hubbard et al, *Experimental Thermochemistry*, Chap. 5, pp. 75-128. F. D. Rossini, editor. Interscience: 1956.

[b] $\varepsilon^i(cont)(t_i - 298.15\ K) + \varepsilon^f(cont)(298.15\ K - t_f + \Delta t_{corr})$.

[c] Items 81 to 85, 87 to 90, 93 and 94 of the computation form of Hubbard et al (footnote a).

TABLE 6. Summary of Combustion Experiments for JP-4-S-A(UN-81-141) and JP-4-S-U(UN-81-149) fuels[a]

(cal_{th} = 4.184 J)

Sample	JP-4-S-A(UN-81-141)			JP-4-S-U(UN-81-149)		
Experiment number	1	2	3	1	2	3
m'(fuel)/g	0.667500	0.673418	0.671975	0.660780	0.680387	0.653276
m''(auxiliary oil)/g	0.053899	0.050716	0.053975	0.069630	0.039719	0.071866
m'''(fuse)/g	0.001055	0.001046	0.001010	0.000799	0.001193	0.001109
$n^i(H_2O)$/mol	0.05535	0.05535	0.05535	0.05535	0.05535	0.05535
$\Delta t_c/K = (t_f - t_i + \Delta t_{corr})/K$	1.98881	2.00023	2.00481	2.02651	2.00216	2.01577
ε(calor)$(-\Delta t_c)/cal_{th}$	-7969.70	-8015.47	-8033.84	-8120.78	-8023.21	-8077.76
ε(cont)$(-\Delta t_c)/cal_{th}$[b]	-8.67	-8.71	-8.75	-8.90	-8.65	-8.73
$\Delta E_{ign}/cal_{th}$	0.18	0.18	0.18	0.18	0.18	0.18
$\Delta E_{dec}(HNO_3)/cal_{th}$	0.00	14.33	14.96	0.00	12.53	14.66
ΔE(corr to std states)/cal_{th}[c]	2.47	2.39	2.40	2.44	2.32	2.33
$\{-m''(\Delta E_c^\circ/m)$(auxiliary oil)$\}/cal_{th}$	593.13	558.10	593.96	766.23	437.08	790.84
$\{-m'''(\Delta E_c^\circ/m)$(fuse)$\}/cal_{th}$	4.27	4.23	4.09	3.23	4.83	4.49
$\{m'(\Delta E_c^\circ/m)$(fuel)$\}/cal_{th}$	-7378.32	-7444.95	-7427.00	-7357.60	-7574.92	-7273.99
$\{(\Delta E_c^\circ/m)$(fuel)$\}/cal_{th}\ g^{-1}$	-11053.66	-11055.46	-11052.50	-11134.70	-11133.24	-11134.65
$\{(\Delta E_c^\circ/m)$(fuel)$\}/cal_{th}\ g^{-1}$	-11053.87 ± 0.86 (mean and standard deviation of the mean)			-11134.20 ± 0.48		

[a] The symbols and abbreviations of this table are those of W. N. Hubbard et al, *Experimental Thermochemistry*, Chap. 5, pp. 75-128. F. D. Rossini, editor. Interscience: 1956.

[b] ε^i(cont)$(t_i - 298.15\ K) + \varepsilon^f$(cont)$(298.15\ K - t_f + \Delta t_{corr})$.

[c] Items 81 to 85, 87 to 90, 93 and 94 of the computation form of Hubbard et al (footnote a).

TABLE 7. Summary of combustion experiments for JP-4-S-S(UN-81-155) and JP-4P-TK-F2 fuels[a]

(cal_{th} = 4.184 J)

Sample	JP-4-S-S(UN-81-155)				JP-4P-TK-F2		
Experiment number	1	2	3	4	1	2	3
m'(fuel)/g	0.635793	0.651134	0.623469	0.594547	0.633889	0.644861	0.651471
m''(auxiliary oil)/g	0.067031	0.068983	0.096102	0.124989	0.051761	0.081177	0.070461
m'''(fuse)/g	0.000928	0.001206	0.001209	0.001014	0.000987	0.001081	0.001008
$n^i(H_2O)$/mol	0.05535	0.05535	0.05535	0.05535	0.05535	0.05535	0.05535
$\Delta t_c/K = (t_f - t_i + \Delta t_{corr})/K$	1.95521	2.00736	2.00441	2.00304	1.90235	2.01664	2.00617
ϵ(calor)$(-\Delta t_c)/cal_{th}$	-7835.07	-8044.06	-8032.20	-8026.71	-7623.23	-8081.23	-8039.27
ϵ(cont)$(-\Delta t_c)/cal_{th}$[b]	-8.50	-8.71	-8.72	-8.75	-8.18	-8.82	-8.70
$\Delta E_{ign}/cal_{th}$	0.18	0.18	0.18	0.18	0.18	0.18	0.18
$\Delta E_{dec}(HNO_3)/cal_{th}$	0.00	14.89	14.71	13.56	0.00	13.95	12.52
ΔE(corr to std states)$/cal_{th}$[c]	2.30	2.28	2.28	2.29	2.23	2.32	2.31
$\{-m''(\Delta E_c^\circ/m)$(auxiliary oil)$\}/cal_{th}$	737.63	759.12	1057.55	1375.43	569.59	893.31	775.38
$\{-m'''(\Delta E_c^\circ/m)$(fuse)$\}/cal_{th}$	3.76	4.88	4.90	4.11	4.00	4.38	4.08
$\{m'(\Delta E_c^\circ/m)$(fuel)$\}/cal_{th}$	-7099.70	-7271.42	-6961.30	-6639.89	-7055.41	-7175.91	-7253.50
$\{(\Delta E_c^\circ/m)$(fuel)$\}/cal_{th}\ g^{-1}$	-11166.68	-11167.33	-11165.44	-11167.99	-11130.35	-11127.86	-11134.04
$\{(\Delta E_c^\circ/m)$(fuel)$\}/cal_{th}\ g^{-1}$	-11166.86 ± 0.54 (mean and standard deviation of the mean)				-11130.75 ± 1.89		

[a] The symbols and abbreviations of this table are those of W. N. Hubbard et al, *Experimental Thermochemistry*, Chap. 5, pp. 75-128. F. D. Rossini, editor. Interscience: 1956.

[b] ϵ^i(cont)$(t_i - 298.15\ K) + \epsilon^f$(cont)$(298.15\ K - t_f + \Delta t_{corr})$.

[c] Items 81 to 85, 87 to 90, 93 and 94 of the computation form of Hubbard et al (footnote a).

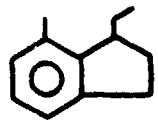
TABLE 8. Properties summary

Sample designation	Empirical formula [a]	Density 15°C [b] g cm^{-3}	Density 25°C	$\Delta E_c^\circ/m$ Eq. 2 cal g^{-1} [c]	Deviation Eq. 3 [d]
BP-IP-1	$CH_{1.9696}$	0.7989	0.795	-10337.4	-6.6
BP-IP-2	$CH_{1.9589}S_{0.0006}$	0.7888	0.785	-10319.6	-1.1
BP-IP-3	$CH_{1.9487}S_{0.0011}$	0.7948	0.791	-10298.2	-8.1
BP-IP-4	$CH_{1.9397}S_{0.0009}$	0.8002	0.797	-10304.9	-4.1
BP-IP-5	$CH_{1.9089}$	0.7990	0.791	-10295.1	-14.7
BP-IP-6	$CH_{1.8604}S_{0.0001}$	0.8293	0.826	-10231.6	5.3
BP-IP-7	$CH_{1.8675}$	0.8180	0.814	-10246.6	-2.9
BP-IP-9	$CH_{1.7784}S_{0.0001}$	0.8309	0.824	-10179.6	-8.0
JP-10	$CH_{1.6806}$ [e]	0.9193	0.918	-10071.2	10.6
JP-7P-TK-WA-10	$CH_{2.0258}$ [e]	0.7994	0.793	-10376.7	0.3
JP-4-S-A(UN-81-141)	$CH_{1.9630}$	0.7825	0.780	-10315.9	-0.1
JP-4-S-U(UN-81-149)	$CH_{2.0188}S_{0.0004}$	0.7801	0.779	-10376.9	-5.3
JP-4-S-S(UN-81-155)	$CH_{2.0475}$ [e]	------	0.758	-10401.7	-7.0
JP-4P-TK-F2	$CH_{2.0444}S_{0.0001}$	------	0.759	-10366.3	25.7

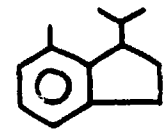
[a] From analysis for each element.
[b] From Wright-Patterson Air Force Base.
[c] 1 cal = 4.184 J.
[d] Deviation of $\Delta E_c^\circ/m$ from equation 3.
[e] From analysis for carbon only.

2. MODEL COMPOUND STUDIES

No model compounds were studied this year; however, samples of 1-isopropyl-7-methylindan and 1-ethyl-7-methylindan were recently received from the laboratories of E. J. Eisenbraun at Oklahoma State University where the compounds were synthesized and purified.



1-Ethyl-7-methylindan



1-Isopropyl-7-methylindan

Preparations are being made to study these compounds to further delineate the steric interaction energies of the 1-7-substituted indans in relation to other results for the 1-6-substituted indans and the 1-8-substituted naphthalenes.[7-10]

3. PUBLICATION AND PRESENTATION

Chemical Thermodynamic Properties of Molecules Which Undergo Inversion: I. Aniline, Methylamine, Cyclopropylamine, and Cyclopentene by J. A. Draeger, R. H. Harrison and W. D. Good. Accepted for publication by the *Journal of Chemical Thermodynamics*.

Thermodynamics of Organic Compounds by W. D. Good and N. K. Smith was presented at the AFOSR meeting on Airbreathing Combustion Dynamics at Clearwater, Florida, November 16-20, 1981.

REFERENCES

1. Good, W. D. *J. Chem. Eng. Data*, v. 14, 1969, pp. 231-235.
2. Good, W. D., and N. K. Smith. *J. Chem. Eng. Data*, v. 14, 1969, pp. 102-106.
3. Good, W. D., D. W. Scott, and G. Waddington. *J. Phys. Chem.*, v. 60, 1956, pp. 1080-1089.
4. Good, W. D., D. R. Douslin, D. W. Scott, A. George, J. L. Lacina, J. P. Dawson, and G. Waddington. *J. Phys. Chem.*, v. 63, 1959, pp. 1133-1138.
5. Guthrie, G. B., Jr., D. W. Scott, W. N. Hubbard, C. Katz, J. P. McCullough, M. E. Gross, K. D. Williamson, and G. Waddington. *J. Am. Chem. Soc.*, v. 74, 1952, pp. 4662-4669.
6. Wagman, D. D., W. H. Evans, I. Halow, V. B. Parker, S. M. Bailey, and R. H. Schumm. *Natl. Bur. Stds. (U.S.) Tech. Note 270-3*, 1968, pp. 1-264.

7. AFOSR Final Technical Summary Report, 1976-1977.
8. W. D. Good. *J. Chem. Thermodynamics*, v. 5, 1973, pp. 715-720.
9. AFOSR Final Technical Summary Report, 1979-1980.
10. AFOSR Final Technical Summary Report, 1980-1981.

DISTRIBUTION LIST

CONTRACTORS

Aerospace Corporation
The Ivan L Getting Laboratories
Attn: Dr Charles M Randall
P O Box 95085
Los Angeles, CA 90045

CINDAS
Purdue University Research Park
Attn: Dr H H Li
2595 Yeager Road
West Lafayette, IN 47907

Department of Energy
Bartlesville Energy Technology Center
Attn: Mr William D Good
Bartlesville, OK 74003

Dow Chemical Company
Thermal Laboratory, Bldg 1707
Attn: Dr Malcolm Chase
Midland, MI 48640

University of Manchester/UMIST
Department of Metallurgy
Attn: Dr Roy Taylor
Grosvenor Street
Manchester M1 7HS, ENGLAND

Department of Energy
Pittsburgh Energy Technology Center
Attn: Dr Francis E Spencer, Jr
P. O. Box 10940
Pittsburgh, PA 15236

National Bureau of Standards
Thermophysics Division
Attn: Dr Ared Cezairliyan
Washington, DC 20234

National Bureau of Standards
Chemical Thermodynamics Division
Attn: Dr Stan Abramowitz
Mr David Ditmars
Washington, DC 20234

University of Nevada
Mackay School of Mines
Attn: Prof Eugene Miller
Reno, NV 89507

Purdue University
School of Mechanical Engineering
Properties Research Laboratory
Attn: Dr R E Taylor
2595 Yeager Road
West Lafayette, IN 47907

Space Sciences, Inc
Attn: Mr Milton Farber
135 W Maple
Monrovia, CA 91016

SRI International
Physical Sciences Division
Attn: Dr D L Hildenbrand
Menlo Park, CA 94025

NON-CONTRACTORS

AFML/MXE (L Scott Theibert)
Wright-Patterson AFB, OH 45433

AFML/LP (Dr Merrill L Minges)
Wright-Patterson AFB, OH 45433

AFML/MBC (Dr W C Kessler)
Wright-Patterson AFB, OH 45433

Jet Propulsion Laboratory
Attn: Mr. Theodore W Price
4800 Oak Grove Drive
Pasadena, CA 91103

Johns Hopkins University
Applied Physics Laboratory
Attn: Dr Robert Fristrom
Johns Hopkins Road
Laurel, MD 20810

NON-CONTRACTORS--Continued

AFRPL/LKCB (Mr Curtis C Selph)
Edwards AFB, CA 93523

AFRPL/PACP (Dr David Mann)
Edwards AFB, CA 93523

AFWL/ALD (Dr Leroy Wilson)
Kirtland AFB, NM 87117

AFWL/ALD (Major David S Olson)
Kirtland AFB, NM 87117

AFAOL/RJT (Dr F D Stull)
Wright-Patterson AFB, OH 45433

U.S. Army Research Office
Attn: Dr David R Squire
P O Box 12211
Research Triangle Park, NC 27709

Atlantic Research Corporation
Attn: Dr Charles Henderson
5390 Cherokee Avenue
Alexandria, VA 22314

University of California
Department of Chemistry
Attn: Dr Leo Brewer
Berkeley, CA 94700

Cornell University
Department of Chemistry
Attn: Dr S H Bauer
Ithica, NY 14850

NSSC
Department of the Navy
Code NSEA-0331
Attn: Mr John W Murrin
Washington, DC 20360

Naval Ordnance Station
Attn: Mr Al Camp
Indian Head, MD 20640

NASA
Lewis Laboratories (Mail Stop 6-1)
Attn: Mr Sanford Gordon
Cleveland, OH 44135

NAS-NRC
Numerical Data Advisory Board
2101 Constitution Avenue, NW
Washington, DC 20418

National Bureau of Standards
OSRD
Attn: Dr David Lide
Washington, DC 20234

National Bureau of Standards
Chemical Thermodynamics Division
Attn: Mr Donald D Wagman
Washington, DC 20234

National Bureau of Standards
Office of Standard Reference
Materials
Attn: Dr Richard Kirby
Washington, DC 20234

National Bureau of Standards
Thermophysical Properties Division
Attn: Dr Jerry Hust
Boulder, CO 80302

Office of Naval Research
Attn: Mr Rudolph Marcus
1030 E Green Street
Pasadena, CA 91101

Office of Naval Research
Power Program, Code 473
Attn: Dr Richard Miller
800 North Quincy Street
Arlington, VA 22217

Rice University
Department of Chemistry
Attn: Dr John Margrave
Houston, TX 77001

United Technologies Corporation
Chemical Systems Division
Attn: Dr R O MacLaren
Sunnyvale, CA 94086

Chemical Propulsion Information
Agency
APL/JHU (2 copies)
Johns Hopkins Road
Laurel, MD 20810